

APPENDIX

Metabolomics Insights in Early Childhood Caries

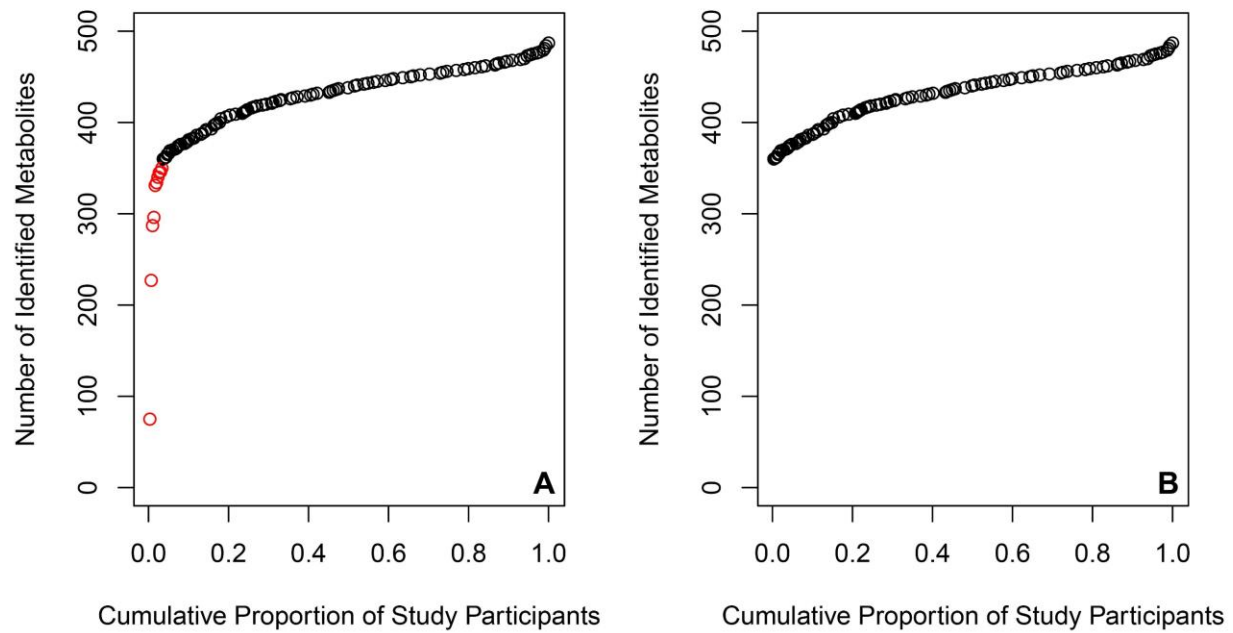
Heimisdottir LH,¹ Lin BM,² Cho H,² Orlenko A,³ Ribeiro AA,⁴ Simon-Soro A,⁵⁻⁷ Roach J,⁸
Shungin D,^{9,10} Ginnis J,¹ Simancas-Pallares MA,¹ Spangler HD,¹ Ferreira Zandona AG,¹¹ Wright
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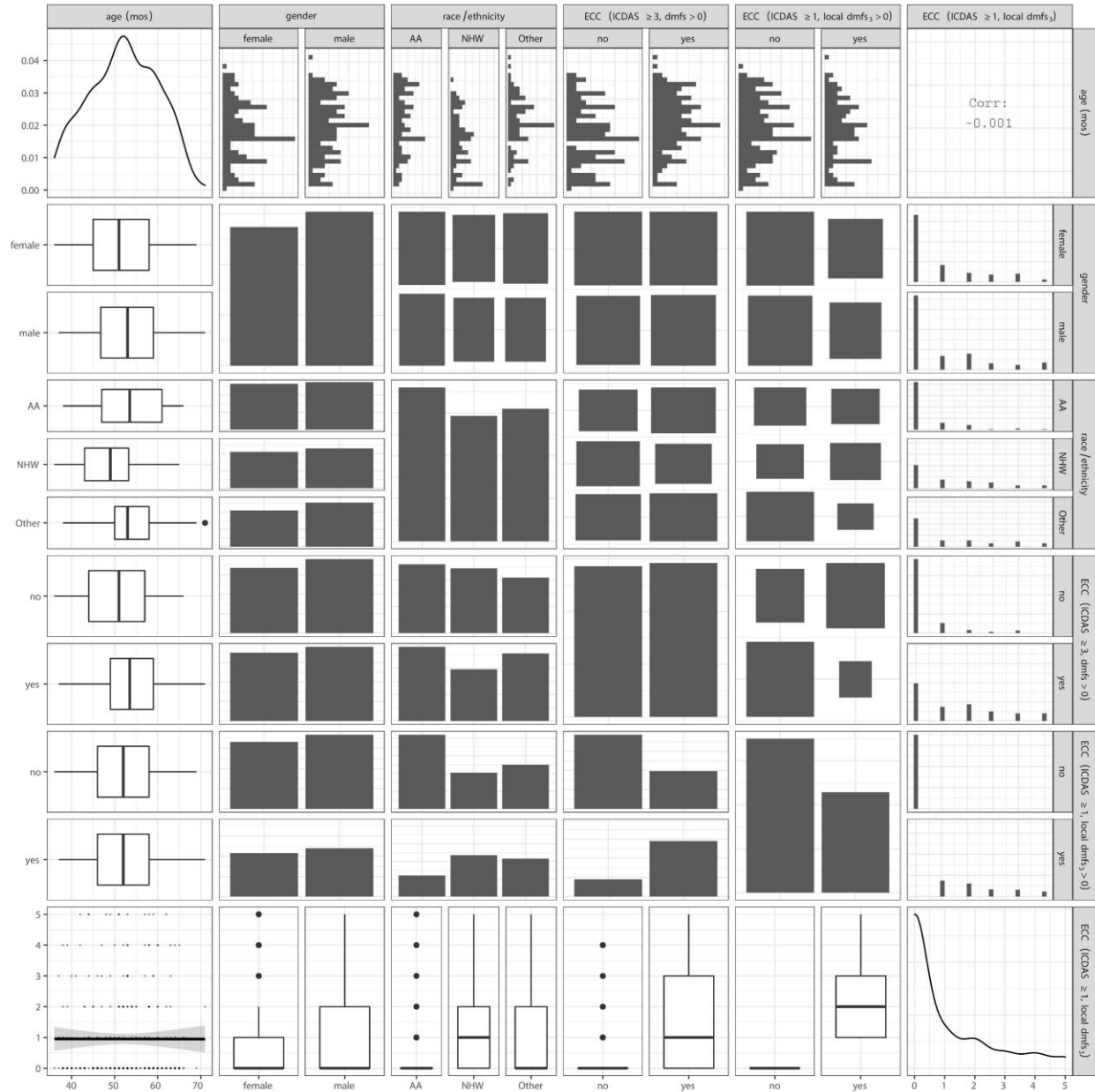
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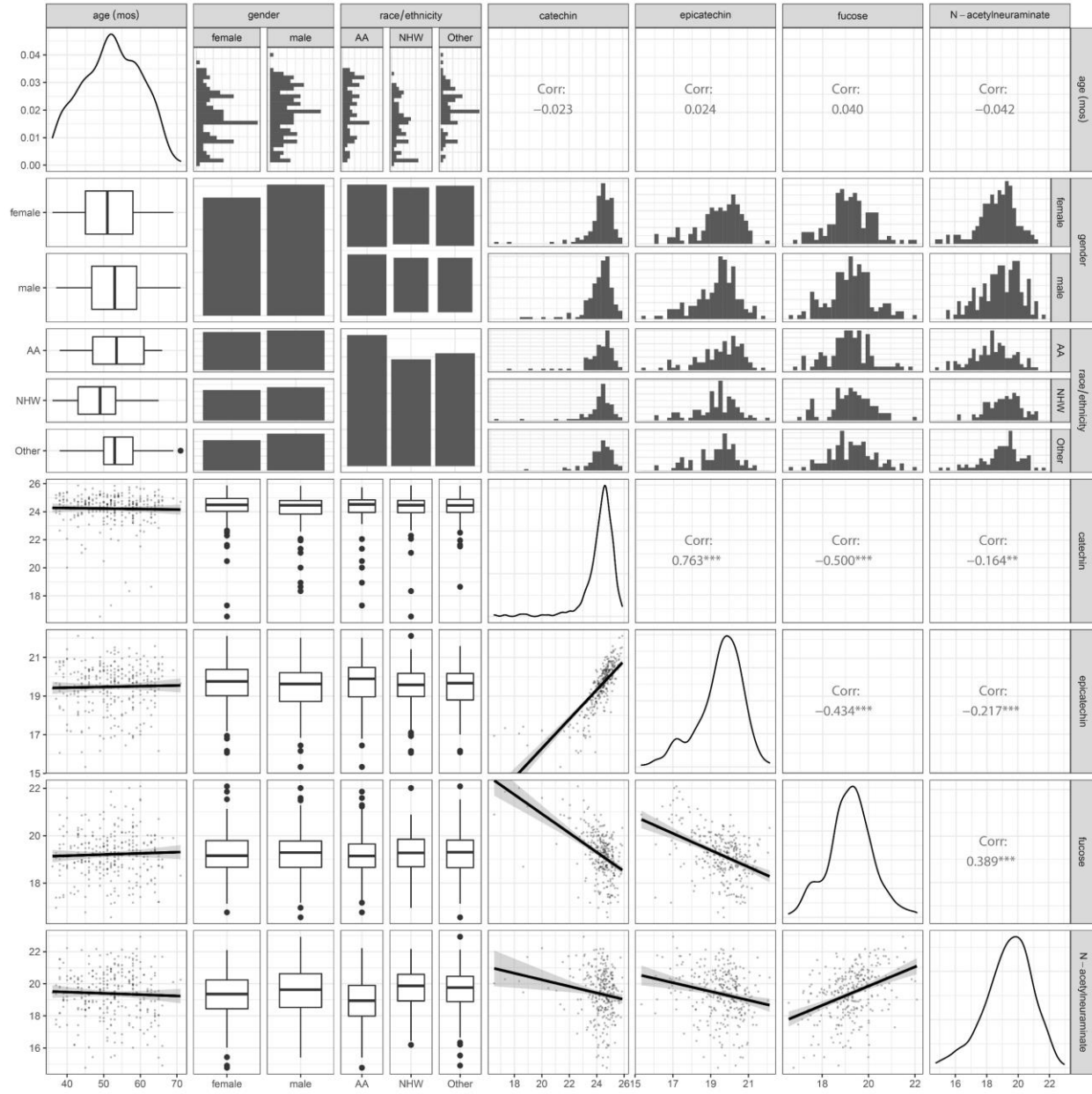
APPENDIX FIGURES



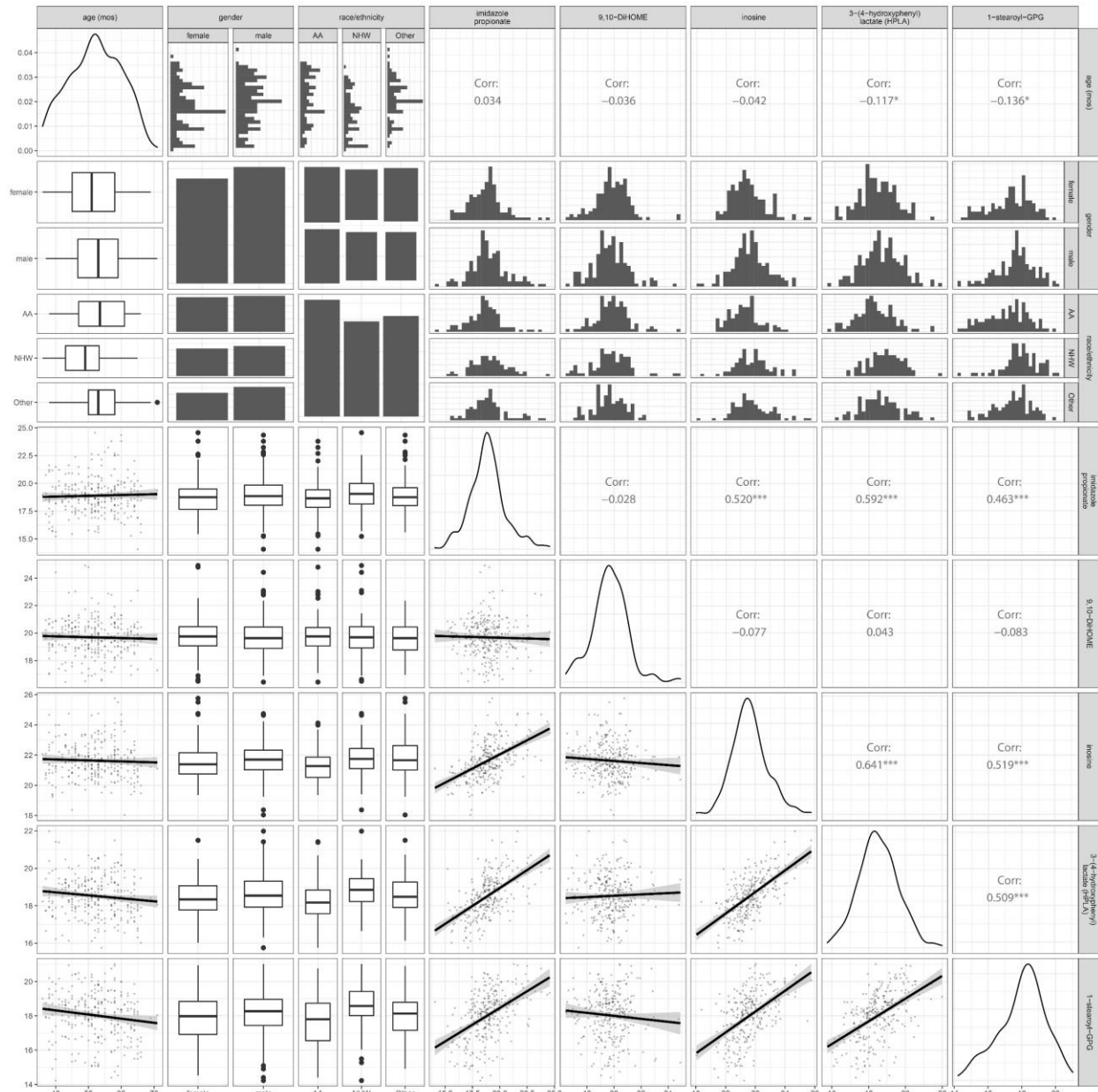
Appendix Figure 1. Distribution of participant-level metabolite missingness in the study sample (panel A). Individuals with >30% missingness (n=10, marked red; 3 early childhood caries ‘cases’ and 7 ‘controls’) were excluded from analyses (panel B).



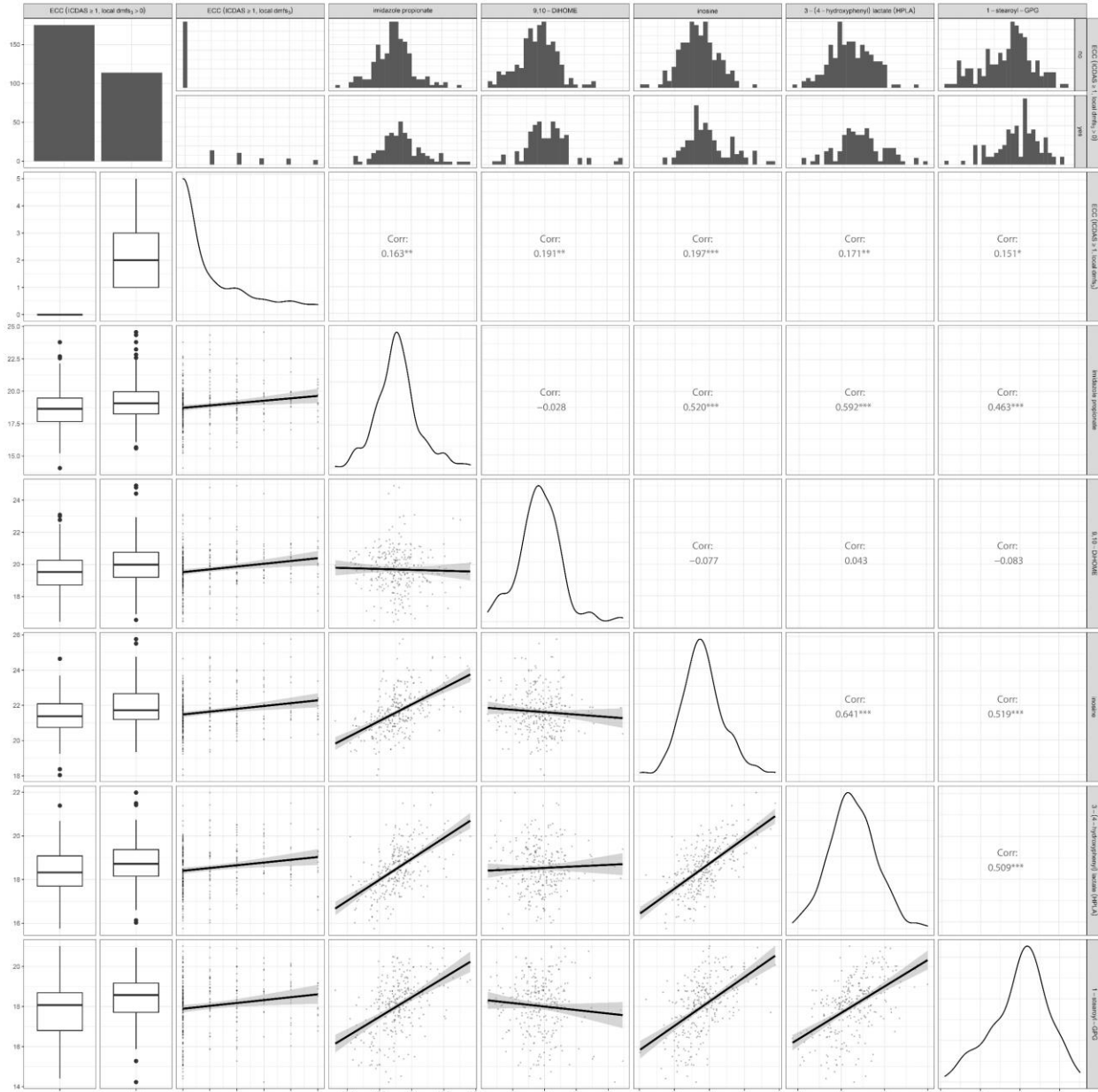
Appendix Figure 2. Distribution of participants' demographic characteristics (age, gender, and race/ethnicity) and the two ECC localized experience traits (localized dmfs₃ index, defined at the ICDAS_≥1 threshold) and prevalence (localized dmfs₃>0 vs. dmfs₃=0, defined at the ICDAS_≥1 threshold), and the person-level ECC trait (person-level dmfs>0, defined at the ICDAS_≥3 threshold) that demonstrated statistically significant associations with metabolites.



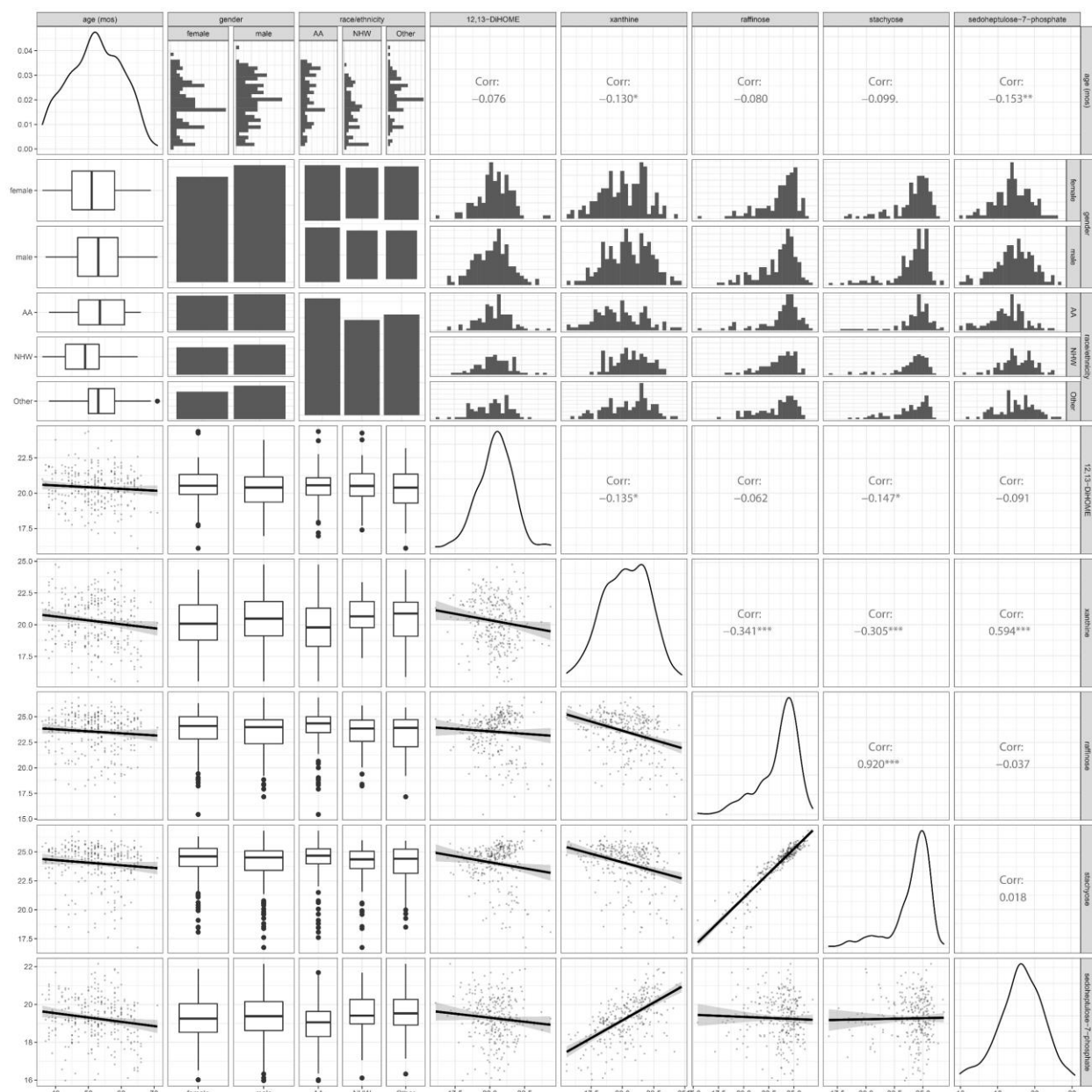
Appendix Figure 3. Distribution of metabolites found to be statistically significantly altered after FDR correction ($q < 0.05$) in 2 ECC experience trait analyses: catechin, epicatechin, fucose and N-acetylneuraminate abundances are presented over participants' demographic characteristics.



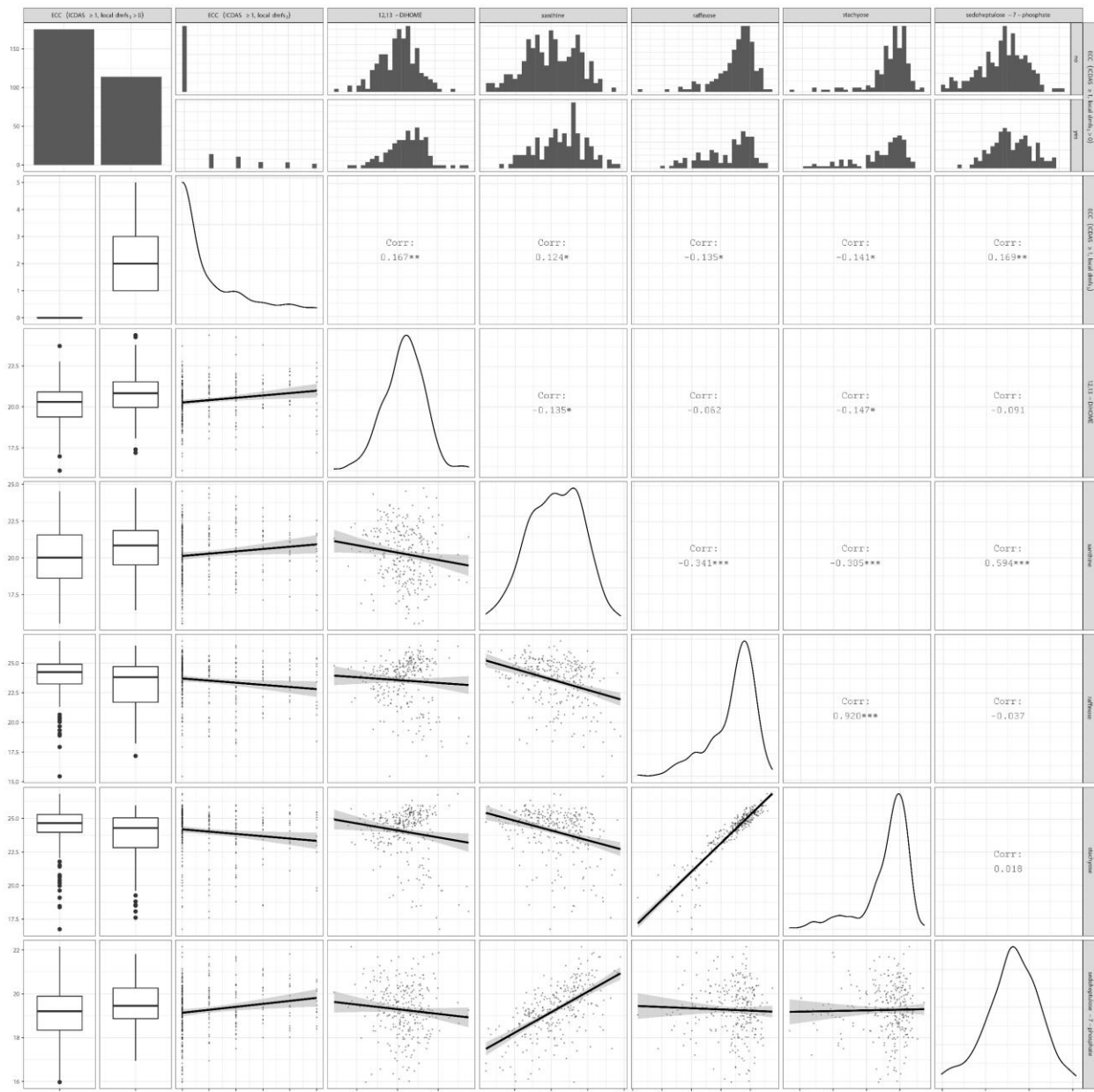
Appendix Figure 5. Distribution of metabolites found to be statistically significantly altered after FDR correction ($q < 0.05$) in 1 ECC localized experience trait analysis: imidazole propionate, 9,10-DiHOME, inosine, 3-(4-hydroxyphenyl) lactate (HPLA), and 1-stearoyl-GPG abundances are presented over participants' demographic characteristics.



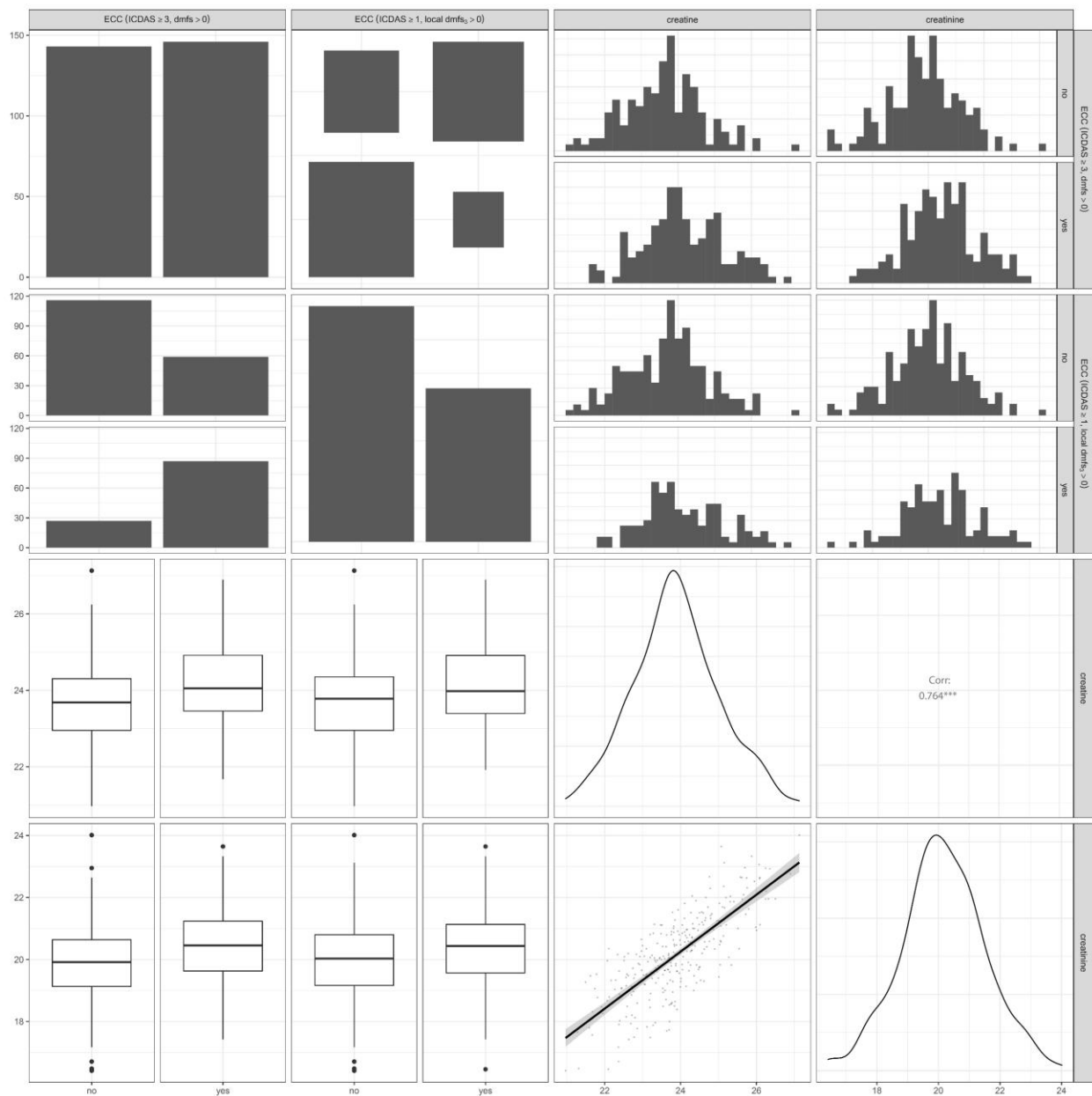
Appendix Figure 6. Distribution of metabolites found to be statistically significantly altered after FDR correction ($q < 0.05$) in 1 ECC localized experience trait analysis: imidazole propionate, 9,10-DiHOME, inosine, 3-(4-hydroxyphenyl) lactate (HPLA), and 1-stearoyl-GPG abundances are presented over ECC experience (localized $dmfs_3$ index, defined at the $ICDAS \geq 1$ threshold) and prevalence (localized $dmfs_3 > 0$ vs. $dmfs_3 = 0$, defined at the $ICDAS \geq 1$ threshold).



Appendix Figure 7. Distribution of metabolites found to be statistically significantly altered after FDR correction ($q < 0.05$) in 1 ECC localized experience trait analysis: 12,13-DiHOME, xanthine, raffinose, stachyose, sedoheptulose-7-phosphate abundances are presented over participants' demographic characteristics.



Appendix Figure 8. Distribution of metabolites found to be statistically significantly altered after FDR correction ($q < 0.05$) in 1 ECC localized experience trait analysis: 12,13-DiHOME, xanthine, raffinose, stachyose, sedoheptulose-7-phosphate abundances are presented over ECC experience (localized $dmfs_3$ index, defined at the $ICDAS \geq 1$ threshold) and prevalence (localized $dmfs_3 > 0$ vs. $dmfs_3 = 0$, defined at the $ICDAS \geq 1$ threshold).



Appendix Figure 9. Distribution of the two metabolites (creatine and creatinine) that were found to be statistically significantly associated with the person-level ECC trait (person-level dmfs>0, defined at the ICDAS \geq 3 threshold) after FDR correction ($q<0.05$).